=> d his

(FILE 'HOME' ENTERED AT 14:07:50 ON 21 JAN 2004)

FILE 'REGISTRY' ENTERED AT 14:08:33 ON 21 JAN 2004
L1 1 S 2582-30-1/RN

FILE 'CAPLUS' ENTERED AT 14:08:48 ON 21 JAN 2004
L2 366 S L1
L3 25 S L2 AND CRYSTAL?
L4 0 S L3 AND DIAMETER

=> d l3 bib abs 1-25

L3 ANSWER 1 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:609454 CAPLUS
DN 139:388758
TI 4,5-Dihydro-3-methyl-5-(4-methylphenyl)-1H-pyrazole-1-carboxamide
AU Kettmann, Viktor; Svetlik, Jan
CS Faculty of Pharmacy, Comenius University, Bratislava, 83232, Slovakia
SO Acta Crystallographica, Section C: Crystal Structure Communications (2003), C59(8), o419-o421
CODEN: ACSCEE; ISSN: 0108-2701
PB Blackwell Publishing Ltd.
DT Journal
LA English
AB The reaction between 4-(4-methylphenyl)but-3-en-2-one and aminoguanidine produced an unexpected product C12H15N3O, consisting of a carboxamide moiety joined to a substituted pyrazoline ring at one of the N atoms. The pyrazoline ring adopts a flat-envelope conformation and the substituted Ph ring is oriented almost perpendicular to the heterocycle. The carbonyl O atom has partial anionic character as a result of the transfer of .pi. d. from the two adjacent sp2 N atoms and is involved in an intermol. H bond with the amide group. **Crystallog**. data are given.
RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:455033 CAPLUS
DN 139:41802
TI Stabilized pharmaceuticals containing HMG-CoA reductase inhibitors
IN Pflaum, Zlatko; Kerc, Janez
PA Slovenia
SO U.S. Pat. Appl. Publ., 16 pp., Cont.-in-part of U. S. Ser. No. 591,322.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 3

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2003109584	A1	20030612	US 2002-298187	20021115
US 6531507	B1	20030311	US 2000-591322	20000609
PRAI US 2000-591322	A2	20000609		

AB Lovastatin, pravastatin, simvastatin, mevastatin, atorvastatin, and derivs. and analogs thereof are known as HMG-CoA reductase inhibitors and are used as antihypercholesterolemic agents. The majority of them are produced by fermn. using microorganisms of different species identified as species belonging to Aspergillus, Monascus, Nocardia, Amycolatopsis, Mucor or Penicillium genus, and some are obtained by treating the fermn. products using the methods of chem. synthesis or they are the products of total chem. synthesis. The aforementioned active substances may be destabilized by the environmental factors, their degrdn. may also be accelerated by interactions with other pharmaceutical ingredients, such as

fillers, binders, lubricants, glidants and disintegrating agents, therefore the pharmaceutical ingredients and the process for prepn. of the pharmaceutical formulation should be meticulously chosen to avoid the aforementioned undesired interactions and reactions. The present invention relates to a HMG-CoA reductase inhibitor which is stabilized by forming a homogeneous compn. with a buffering substance or a basifying substance. This homogeneous compn. is suitably used as the active substance in a pharmaceutical formulation for the treatment of hypercholesterolemia and hyperlipidemia. Pravastatin Sodium (5 g) with chromatog. purity 99.5% and pH 7.4 (1%)/7.7 (5%) was dissolved in MeOH (30 mL), and Na2CO3 (10 mg, dissolved in 0.15 mL of water) was added and finally, EtOAc (400 mL contg. 2% of water) was added. Fter 1 h the resulted **crystals** were filtered off, washed with fresh EtOAc (50 mL) and dried at 40.degree. for 6 h in vacuo. The chromatog. purity of resulting **crystals** (4.3 g) was 99.6%.

L3 ANSWER 3 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:196949 CAPLUS
DN 138:226745
TI HMG-CoA reductase inhibitors stabilized by a buffer or basifying substance
IN Pflaum, Zlatko; Kerc, Janez
PA LEK Pharmaceuticals D.D., Slovenia
SO U.S., 12 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6531507	B1	20030311	US 2000-591322	20000609
	AU 2000049434	A5	20011217	AU 2000-49434	20000609
	US 2003109584	A1	20030612	US 2002-298187	20021115
PRAI	US 2000-591322	A	20000609		
	WO 2000-IB773	A	20000609		

AB The present invention relates to a HMG-CoA reductase inhibitor which is stabilized by forming a homogeneous compn. with a buffering substance or a basifying substance. This homogeneous compn. is suitably used as the active substance in a pharmaceutical formulation for the treatment of hypercholesterolemia and hyperlipidemia. Pravastatin Na is stabilized by addn. of Na2CO3.
RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

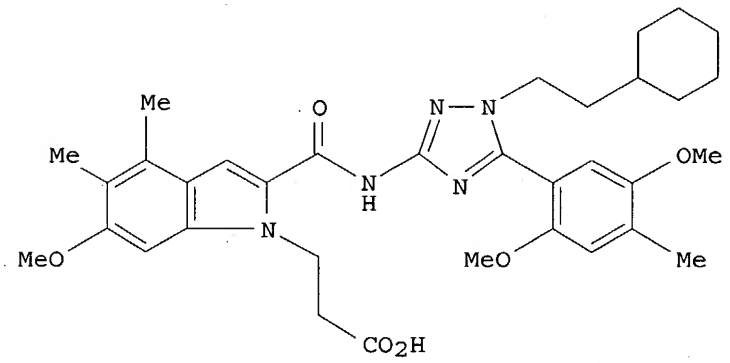
L3 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:332186 CAPLUS
DN 136:340684
TI Preparation and characterization of an indolyl-carboxamido-triazole, polymorphs and solvates thereof as CCK receptor ligands
IN Bignon, Eric; Csikos, Eva; Frehel, Daniel; Goenczi, Csaba; Heja, Gergely; Morvai, Miklos; Podanyi, Benjamin; Varkonyine Schlovicsko, Erika
PA Sanofi-Synthelabo, Fr.
SO PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002034743	A1	20020502	WO 2001-EP12984	20011025
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,				

	US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,				
	DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,				
	BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	FR 2815963	A1	20020503	FR 2000-13728	20001026
	FR 2815963	B1	20030228		
	AU 2002026330	A5	20020506	AU 2002-26330	20011025
	EE 200300161	A	20030616	EE 2003-161	20011025
	EP 1335914	A1	20030820	EP 2001-988716	20011025
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				
	IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	NO 2003001841	A	20030619	NO 2003-1841	20030424
	HR 2003000330	A1	20030630	HR 2003-330	20030428
PRAI	FR 2000-13728	A	20001026		
	HU 2000-4153	A	20001026		
	WO 2001-EP12984	W	20011025		

OS CASREACT 136:340684

GI



I

AB Compd. I and polymorphs, hydrates and salts thereof were prepd. characterized. Me 3-[2-[[[1-(2-cyclohexylethyl)-5-(2,5-dimethoxy-4-methylphenyl)-1H-1,2,4-triazol-3-yl]amino]carbonyl]-6-methoxy-4,5-dimethyl-1H-indol-1-yl]propanoate (prepd. in 5 steps from 2,5-Dimethoxy-4-methylbenzoic acid) was condensed with 4,5-Dimethyl-6-methoxy-1-(3-methoxy-3-oxopropyl)-1H-indole-2-carboxylic acid (prepd. in 4 steps from Et 4,5-dimethyl-6-methoxy-1H-indole-2-carboxylate) and the resulting ester treated with KOH to provide I.bul.potassium salt (II). II was acidified with HCl to provide the acid which was used to generate the ethanolamine, diethanolamine, 1-adamantanamine and diethylamine salts. Prepns. of at least 6 polymorphs of I were described as well as characterization by XRPD, DSC, IR and solid state 13C-NMR. Polymorphic interconversion was also described. These compds. are powerful and selective CCK1 receptor agonists. I had IC50 = 0.4 nM for CCK1 and 234 nM for the CCK2 receptor.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:9182 CAPLUS
DN 136:225779
TI (CN4H7)2.cntdot.Zn3(HPO3)4, a three-dimensional framework zincophosphite: an example of template-template co-operation?
AU Harrison, William T. A.; Phillips, Mark L. F.; Nenoff, Tina M.
CS Department of Chemistry, University of Aberdeen, Aberdeen, AB24 3UE, UK
SO International Journal of Inorganic Materials (2001), 3(7), 1033-1038
CODEN: IJIMCR; ISSN: 1466-6049
PB Elsevier Science Ltd.
DT Journal

LA English
AB The hydrothermal synthesis and single **crystal** structure of (CN4H7)2.cntdot.Zn3(HPO3)4 are reported. This phase is built up from a network of vertex-linked ZnO4 and HPO3 building units encapsulating the extra-framework aminoguanidinium cations. A new type of three-dimensional network for the inorg. component of the structure arises, which contains polyhedral 4-, 6-, 8-, 12- and 16-rings. There are close (.apprx.3.6 .ANG.), side-on, template-template contacts similar to those seen between pairs of guanidinium cations in mol. compds. **Crystal** data: (CN4H7)2.cntdot.Zn3(HPO3)4, Mr = 666.30, monoclinic, space group P21/n, a 10.2589(4), b 29.5851(12), c 13.7578(5) .ANG., .beta. 103.303(1).degree., Z = 8, T = 298(2) K, R = 0.0399, wR(F2)=0.0792.
RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:903840 CAPLUS
DN 136:25125
TI Stabilized pharmaceutical compositions of statin derivs. as HMG-CoA reductase inhibitors
IN Pflaum, Zlatko; Kere, Janez
PA Lek Pharmaceutical and Chemical Company D.D., Slovenia
SO PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001093860	A1	20011213	WO 2000-IB773	20000609
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 2000049434	A5	20011217	AU 2000-49434	20000609
	EP 1292293	A1	20030319	EP 2000-931486	20000609
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
	JP 2004501121	T2	20040115	JP 2002-501433	20000609
	NO 2002005784	A	20021202	NO 2002-5784	20021202
PRAI	US 2000-591322	A	20000609		
	WO 2000-IB773	A	20000609		

AB Lovastatin, pravastatin, simvastatin, mevastatin, atorvastatin, and derivs. and analogs thereof are known as HMG-CoA reductase inhibitors and are used as antihypercholesterolemic agents. The majority of them are produced by fermn. using microorganisms of different species identified as species belonging to Aspergillus, Monascus, Nocardia, Amycolatopsis, Mucor or Penicillium genus, and some are obtained by treating the fermn. products using the methods of chem. synthesis or they are the products of total chem. synthesis. The aforementioned active substances may be destabilized by the environmental factors, their degrdn. may also be accelerated by interactions with other pharmaceutical ingredients, such as fillers, binders, lubricants, glidants and disintegrating agents, therefore the pharmaceutical ingredients and the process for prepn. of the pharmaceutical formulation should be meticulously chosen to avoid the aforementioned undesired interactions and reactions. The present invention relates to a HMG-CoA reductase inhibitor which is stabilized by forming a homogeneous compn. with a buffering substance or a basifying substance. This homogeneous compn. is suitably used as the active

substance in a pharmaceutical formulation for the treatment of hypercholesterolemia and hyperlipidemia. Pravastatin Na is stabilized by addn. of Na carbonate.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:779792 CAPLUS
DN 136:102081
TI Vibrational and theoretical study of the protonation of 3,4'-bi-1,2,4-triazole and its C-brominated and C-methylated derivatives
AU Guedira, F.; Ouijja, N.; Zaydoun, S.; Komiha, N.; Lautie, A.; Idrissi, M. Saidi
CS Laboratoire de Spectroscopie Infrarouge, Departement de Chimie, Faculte des Sciences, Rabat, Morocco
SO Canadian Journal of Analytical Sciences and Spectroscopy (2001), 46(1), 1-9
CODEN: CJASFA; ISSN: 1205-6685
PB Spectroscopy Society of Canada
DT Journal
LA French
AB An approach to det. the structure of protonated 3,4'-di-1,2,4-triazoles was carried out using the semi-empirical M.N.D.O. (MNDO) method. The results obtained for 3,4'-di-1,2,4-triazole show that the isolated state of the N1H form has great stability, and indicated that its protonation mainly occurs on one of the pyridine type N of the 4-triazolyl group. The vibration spectra of the di-1,2,4-triazolium, 5-methyl-di-1,2,4-triazolium and 5-bromo-di-1,2,4-triazolium chlorides were studied between 4000 and 200 cm-1. An attribution of the fundamental modes is proposed, and the effect of protonation on the normal vibration frequencies is discussed. Using these spectroscopic results, the strength and type of H bonds existing in the **crystal** could be assessed and a mol. structure proposed.

RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 8 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:63962 CAPLUS
DN 134:115676
TI Method for making aminoguanidine bicarbonate with particular **crystal** properties from carbon dioxide and aqueous solutions of cyanamide and hydrazine hydrate
IN Bossoutrot, Jean-Michel; Bourdauducq, Paul
PA Atofina, Fr.
SO PCT Int. Appl., 14 pp.
CODEN: PIXXD2
DT Patent
LA French
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001005752	A1	20010125	WO 2000-FR1579	20000608
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	FR 2796378	A1	20010119	FR 1999-9257	19990716
	FR 2796378	B1	20010824		
	EP 1196378	A1	20020417	EP 2000-942170	20000608

EP 1196378 B1 20030820
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO
JP 2003505364 T2 20030212 JP 2001-511413 20000608
AT 247637 E 20030915 AT 2000-942170 20000608
PRAI FR 1999-9257 A 19990716
WO 2000-FR1579 W 20000608
AB Aminoguanidine bicarbonate (I) is prepd. from an aq. soln. of cyanamide and an aq. soln. of hydrazine hydrate in the presence of CO2 using an amt. of cyanamide slightly higher than the stoichiometric quantity.. This method produces I **crystals** which are quasi-spherical agglomerates.
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 9 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:118432 CAPLUS
DN 132:259620
TI Pentafluorosulfanylnitramide Salts
AU Sitzmann, Michael E.; Gilardi, Richard; Butcher, Ray J.; Koppes, William M.; Stern, Alfred G.; Thrasher, Joseph S.; Trivedi, Nirupam J.; Yang, Zhen-Yu
CS Indian Head Division, Naval Surface Warfare Center, Indian Head, MD, 20640, USA
SO Inorganic Chemistry (2000), 39(4), 843-850
CODEN: INOCAJ; ISSN: 0020-1669
PB American Chemical Society
DT Journal
LA English
AB The synthesis and properties of a new class of inorg. salts, named pentafluorosulfanylnitramide salts (or pentafluorosulfanylnitraminic acid salts) [Z+SF5NNO2-], are described. A no. of SF5-nitramide salts (Z+SF5NNO2-) were successfully prepd. via nucleophilic displacements from carbamates and/or ion exchange techniques, but some salts [M(SF5NNO2)x; M = Li, Mg, Al] decompd. during isolation procedures and appear to be unstable in the solid state. Single-**crystal** x-ray diffraction was used to fully characterize the Z+SF5NNO2-, and their properties/structures are compared with those of the corresponding dinitramide salts (or dinitraminic acid salts), Z+N(NO2)2-. X-ray **crystallog**. revealed major structural differences between N(NO2)2- and SF5N(NO2)- salts concerning the N-N distances and the angles subtended at the central N atom. In the N(NO2)2- salts, there are two nonequivalent N-N (av. lengths 1.372(2) and 1.354(2) .ANG.) distances and an av. N-N-N angle of 115.8(3).degree. (falls between sp3 and sp2 hybridization). In the SF5NNO2- salts, the av. N-N distance is much shorter, 1.308(9) .ANG., and the av. N-N-S angle is 120.0(5).degree. (closely fits sp2 hybridization). The SF5NNO2- salts show a remarkable metrical similarity for the SF5 moiety in all structures, indicating a lack of sensitivity to its steric and electronic environment. This is in marked contrast to N(NO2)2-, where there is a wide variation in conformations adopted by these anions which can be related to their environment.
RE.CNT 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 10 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:488239 CAPLUS
DN 131:228629
TI Guanylhydrazones of (hetero)aryl methyl ketones. Structure and reaction with acetic anhydride
AU Gyorgydeak, Zoltan; Holzer, Wolfgang; Mereiter, Kurt
CS Department Organic Chemistry, Lajos Kossuth Univ., Debrecen, H-4010, Hung.
SO Monatshefte fuer Chemie (1999), 130(7), 899-913
CODEN: MOCMB7; ISSN: 0026-9247
PB Springer-Verlag Wien

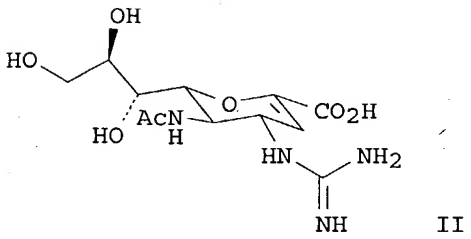
DT Journal
LA English
OS CASREACT 131:228629
AB The synthesis of guanylhydrazones of (hetero)aryl Me ketones is described. Successive reaction with hot Ac2O leads to the corresponding N,N'-diacetyl derivs. Structural assignments of all novel compds. and those of some already known congeners were achieved by NMR (1H, 13C) and x-ray structure anal.
RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 11 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:369050 CAPLUS
DN 131:82130
TI Anhydrous ammonioguanidinium(2+) and dihydrated bis[aminoguanidinium(1+)] hexafluorosilicates: new co-products of preparing ferroelectric ammonioguanidinium(2+) hexafluorozirconate
AU Ross, C. R., II; Bauer, M. R.; Nielson, R. M.; Abrahams, S. C.
CS Department of Structural Biology, St. Jude Children's Research Hospital, Memphis, TN, 38105-2794, USA
SO Acta Crystallographica, Section B: Structural Science (1999), B55(2), 246-254
CODEN: ASBSDK; ISSN: 0108-7681
PB Munksgaard International Publishers Ltd.
DT Journal
LA English
AB Ammonioguanidinium hexafluorosilicate, CH8N42+SiF62-, and bis(aminoguanidinium) hexafluorosilicate dihydrate, 2CH7N4+.cntdot.SiF62-.cntdot.2H2O, are new materials formed as byproducts in course of prepg. ferroelec. CH8N4ZrF6 in the presence of glassware. Their structures were detd. for comparison with the corresponding hexafluorozirconates. All atoms including the eight H atoms in the CH8N42+ cation and the seven H atoms in the CH7N4+ cation were located and refined with wR(F2) = 0.0653, R = 0.0255, S = 1.146 and wR(F2) = 0.0745, R = 0.0301, S = 1.065, resp. The N2C-N-N backbone of the 2+ cation is close to planarity, while that of the 1+ cation does not differ significantly from planarity. The SiF62- octahedron is nearly ideally regular in both materials, with <Si-F> = 1.684 (unbiased estimator of std. uncertainty = 0.016) .ANG. in the anhyd. hexafluorosilicate and 1.6801 (unbiased estimator of std. uncertainty = 0.0006) .ANG. in the dihydrate. The combination of coulombic and NH.cntdot..cntdot..cntdot.F interactions in CH8N4SiF6 results in a relatively dense variant of the NaCl structure. In addn. to similar forces, the dihydrate is also characterized by the role of the water mol. with its strong NH.cntdot..cntdot..cntdot.O interactions; its packing efficiency is, however, appreciably less than that of the anhyd. hexafluorosilicate with an .apprx.8% increase in void space. Cleaved **crystals** of the dihydrate are frequently twinned across the (001) compn. plane, with a 2-fold rotation about the b axis as the twin operation.
RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 12 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:693701 CAPLUS
DN 130:46672
TI Controlled **crystallization** of the gadolinium(III) complex of diethylenetriamine pentaacetate. Monomeric and dimeric structure
AU Ruloff, Robert; Gelbrich, Thomas; Hoyer, Eberhard; Sieler, Joachim; Beyer, Lothar
CS Inst. Anorganische Chemie, Univ. Leipzig, Leipzig, D-04103, Germany
SO Zeitschrift fuer Naturforschung, B: Chemical Sciences (1998), 53(9), 955-959
CODEN: ZNBSEN; ISSN: 0932-0776
PB Verlag der Zeitschrift fuer Naturforschung

DT Journal
LA German
AB The prepn. and x-ray **crystal** structures of 2 Gd(III) complexes of the ligand diethylenetriaminepentaacetic acid (H5dtpa) are reported. With 2 equiv of guanidinium (gu+) per equiv of complex, the dimer (gu)4[Gd2(dtpa)2].(gu)HCO3 (I), and with 1 equiv. of aminoguanidinium (agu+) the monomer (agu)[Gd(Hdtpa)(H2O)].2H2O (II), were obtained, both with the metal atoms in a coordination no. of 9. **Crystal** structures of I: monoclinic, P21/c, a = 15.004(3), b = 10.645(2), c = 17.320(3), .beta. = 102.64(3).degree., V = 2699.3(9) .ANG.3, Z = 2, .rho.c = 1.79 g/cm3, .mu.(MoK.alpha.) = 2.533 mm-1, 5308 independent reflections, 447 refined parameters, R1 = 0.0373, wR2 = 0.1044 (I > 2.sigma.(I)); II: monoclinic, P21/c, a = 15.630(3), b = 17.780(4), c = 17.550(4), .beta. = 91.90(3).degree., V = 4874.5(18) .ANG.3, Z = 8, .rho.c = 1.84 g/cm3, .mu.(MoK.alpha.) = 2.778 mm-1, 9595 independent reflections, 905 refined parameters, R1 = 0.0297, wR2 = 0.0692 (I > 2.sigma.(I)). The dimer contains no coordinated water mol. The monomer is present as 2 **crystallog**. independent complexes H-bridged via carboxylate O atoms (O...O 2.48 .ANG.; O-H...O 172.degree.) and with Gd-Ocoord.water distances of 2.418(4) and 2.423(4) .ANG., resp.
RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 13 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:727381 CAPLUS
DN 128:30045
TI Design and Synthesis of Benzoic Acid Derivatives as Influenza Neuraminidase Inhibitors Using Structure-Based Drug Design
AU Chand, Pooran; Babu, Yarlagadda S.; Bantia, Shanta; Chu, Naiming; Cole, L. Brent; Kotian, Pravin L.; Laver, W. Graeme; Montgomery, John A.; Pathak, Ved P.; Petty, Sandra L.; Shrout, David P.; Walsh, David A.; Walsh, Gerald M.
CS BioCryst Pharmaceuticals Inc., Birmingham, AL, 35244, USA
SO Journal of Medicinal Chemistry (1997), 40(25), 4030-4052
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
GI



II

AB A series of 94 benzoic acid derivs. were synthesized and tested for their ability to inhibit influenza neuraminidase. The enzyme-inhibitor complex structure was detd. by x-ray **crystallog**. anal. for compds. which inhibited the enzyme. The most potent compd. tested in vitro, (4-(acetylamino)-3-guanidinobenzoic acid) (I), had an IC50 = 2.5 .times. 10-6 M against N9 neuraminidase. Compd. I was oriented in the active site of the neuraminidase in a manner that was not predicted from the reported active site binding of GANA (II) with neuraminidase. In a mouse model of influenza, I did not protect the mice from wt. loss due to the influenza virus when dosed intranasally.
RE.CNT 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD

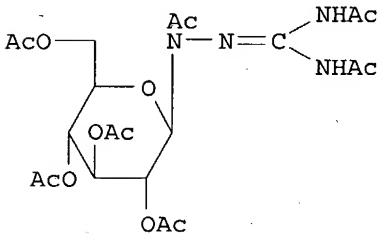
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 14 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:566930 CAPLUS
DN 125:247320
TI **Crystal** and molecular structures of two isomers of phenylglyoxal bis(amidinohydrazone) [phenylglyoxal bis(guanylhydrazone)] sulfate
AU Koskinen, Mikko; Mutikaninen, Ilpo; Elo, Hannu
CS Department Chemistry, University Helsinki, Helsinki, SF-00014, Finland
SO Zeitschrift fuer Naturforschung, B: Chemical Sciences (1996), 51(8), 1161-1172
CODEN: ZNBSEN; ISSN: 0932-0776
PB Verlag der Zeitschrift fuer Naturforschung
DT Journal
LA English
AB A **crystallog**. study on an arom. analog of the antileukemic agent methylglyoxal bis(amidinohydrazone) is reported. Thus, the **crystal** and mol. structures of two different geometrical isomers of phenylglyoxal bis(amidinohydrazone) (I) sulfate were detd. by single-**crystal** x-ray diffraction. **Crystals** were prepd. by recrystg. I sulfate using either H2O or aq. EtOH (vol. ratio EtOH/H2O 1:4) as the solvent. Depending on the solvent, different types of **crystals** were obtained although the I sulfate employed was in both cases from the same synthesis batch that had been prepd. according to classical methods from the glyoxal. When a **crystal** obtained from H2O was studied, I exists solely in the form of the anti-anti isomer, i.e. the same isomer that was obsd. in the cases of all mono- and dialkylglyoxal bis(amidinohydrazones) so far studied. When I sulfate was recrystd. from 20% aq. EtOH, the **crystals** obtained consisted of a different geometrical isomer. In this anti-syn isomer the C:N double bond closest to the Ph group had the syn configuration. In the anti-syn isomer, there is an internal H bond between the two amidinohydrazone moieties, which may markedly contribute to the stabilization of the isomer. The anti-syn isomer of I is analogous to the only isomer of trifluoromethylglyoxal bis(amidinohydrazone) so far obsd. The sulfate of I constitutes the first case in which two different geometrical isomers of a bis(amidinohydrazone) were obsd. The structural flexibility of the bis(amidinohydrazone) chain of I is attributable to the electron-withdrawing resonance effect and perhaps also to the inductive and hyperconjugative effects of the Ph group. The facile isomerization of I may markedly influence the biochem. properties of the compd.

L3 ANSWER 15 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:378959 CAPLUS
DN 125:130793
TI Trinuclear copper(II) coordination compounds with the new ligand 1,9-bis-(3-amino-4H-1,2,4-triazol-5-yl)-3,7-dithianonane; X-ray structures and magnetochemistry
AU Prins, Rob; Biagini-Cingi, Marina; Drillon, Marc; de Graaff, R. A. G.; Haasnoot, Jaap; Manotti-Lanfredi, Anna-Maria; Rabu, Pierre; Reedijk, Jan; Ugozzoli, Franco
CS Leiden Institute of Chemistry, Gorlaeus Laboratories, Leiden University, PO Box 9502, RA Leiden, 2300, Neth.
SO Inorganica Chimica Acta (1996), 248(1), 35-44
CODEN: ICHAA3; ISSN: 0020-1693
PB Elsevier
DT Journal
LA English
AB The syntheses of three new trinuclear Cu(II) complexes with the ligand 1,9-bis-(3-amino-4H-triazol-5-yl)-3,7-dithianonane (attn) are described. The x-ray structures of two of them, [Cu3(attn)2(H2O)2Cl2]Cl4(H2O)4 (1) and [Cu3(attn)2(ZnCl4)2Cl2](H2O)4 (2), were solved. The magnetic properties of these and those of the 3rd related complex, [Cu3(attn)2(H2O)2Br2]Br4(H2O)4 (3), were studied. **Crystallog**.

data: 1: Cu3Cl6C22H52N16O6S4, P.hivin.1, a 8.003(3), b 11.330(4), c 13.072(6) .ANG., .alpha. 112.36(3), .beta. = 90.62(3), .gamma. = 96.64(3).degree., Z = 1, V = 1087(1) .ANG.3, least-squares refinement based on 8956 significant reflections converged to R(Rw) = 0.028 (0.037); 2: Cu3Zn2Cl10C22H48N16O4S4, space group P21/c, a 8.248(5), b 28.203(3), c 10.405(4) .ANG., .beta. 93.07(2).degree., Z = 2, refinement based on 1510 significant reflections converged to R (Rw) = 0.043(0.049); 3 is isomorphous to 1. The structures consist of linear trinuclear units of three Cu(II) ions bridged by two triazole N1N2 bridges and one chloride. The central Cu ion lies on a center of symmetry, coordinated by 4 N and 2 Cl. The coordination distances in .ANG. are: 1: Cu-N = 2.040(1) and 1.985(1), Cu-Cl(bridging) = 2.7390(3); 2: Cu-N = 2.04(1) and 1.98(1), and Cu-Cl(bridging) = 2.878(3). The terminal Cu ions are coordinated by N2S2Cl1O1 (1) and N2S2Cl2 (2), resp. The distances in .ANG. are for 1: Cu-N = 2.003(1) and 2.023(1), Cu-S = 2.3854(3) and 2.3637(3), Cu-Cl(bridging) = 2.5505(3), Cu-O(water) = 2.659(1); for 2: Cu-N = 1.99(1) and 1.98(1), Cu-S = 2.369(4) and 2.390(4), Cu-Cl(bridging) = 2.713(4), Cu-ClZnCl3 = 2.979(5). The shortest Cu-Cu distances within one cluster are 3.5426(1) and 3.620(3) .ANG. for 1 and 2, resp. The magnetic susceptibility data were interpreted from Heisenberg intracluster interactions (J = -75.1, -70.9, -72.3 cm-1 for compds. 1, 2, 3, resp.); a small intercluster exchange (zj' = +1.47, +0.81, +2.03 cm-1 for 1, 2 and 3, resp.) was taken into account in the mean field approxn.

L3 ANSWER 16 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:352408 CAPLUS
DN 122:240264
TI The reaction of D-glucose with aminoguanidine
AU Hirsch, Jan; Petrakova, Eva; Feather, Milton S.; Barnes, Charles L.
CS Department of Biochemistry, University of Missouri, Columbia, MO, 65211, USA
SO Carbohydrate Research (1995), 267(1), 17-25
CODEN: CRBRAT; ISSN: 0008-6215
PB Elsevier
DT Journal
LA English
OS CASREACT 122:240264
GI



I

AB The reaction of D-glucose with aminoguanidine was examd. at pH 7.0 and 37.degree.C (phosphate buffer). Under these conditions, the reaction requires ca. 42 days for 50% of the sugar to react, as measured by the disappearance of D-glucose, and at 60.degree.C all the aminoguanidine had reacted within 72 h. The initial product, a .beta.-D-glucopyranosyl aminoguanidine was obtained in the cryst. state as the trifluoroacetate salt. Data collected on this compd. suggests that, in soln., it is largely a glycosylamine in the .beta. pyranose form. Acetylation gave a cryst. heptaacetate I, which, in soln. (as evidenced by NMR spectroscopy) exists in two different conformational forms. The **crystal** structure of the heptaacetate also includes two conformers. Both **crystallog**. independent mols. are in the normal .beta. pyranose

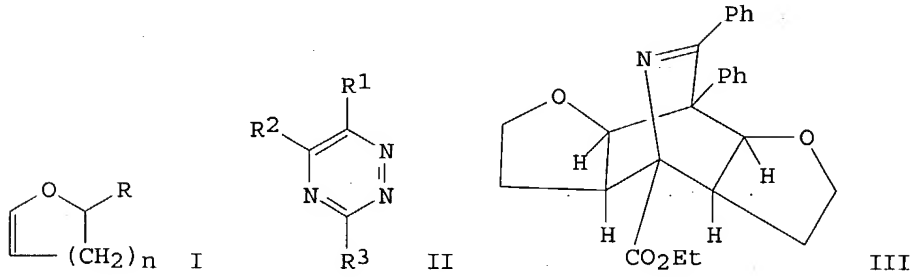
form, with the acetylated guanyl residue occupying different spatial positions relative to the ring.

L3 ANSWER 17 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1994:680064 CAPLUS
DN 121:280064
TI A **crystallographic** study on aminoguanidine dinitrate
AU Mutikainen, I.; Koskinen, M.; Elo, H.
CS Department Chemistry, University Helsinki, Finland
SO Pharmazie (1994), 49(10), 739-42
CODEN: PHARAT; ISSN: 0031-7144
DT Journal
LA English
AB The **crystal** and mol. structure of aminoguanidine dinitrate, CN4H22+.cntdot.(NO3-)2, was detd. with the aid of single-**crystal** X-ray diffraction. In the compd., aminoguanidine dication exists in the form of one tautomer only. One of the pos. charges is localized at the terminal nitrogen atom of the hydrazine part of the dication, while the other is delocalized at the other three nitrogens and obviously also the carbon atom. The dication is remarkably planar. The structure is compared to the corresponding sulfate salt and effects of hydrogen bonding on the planarity of the dication are discussed.

L3 ANSWER 18 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1994:482486 CAPLUS
DN 121:82486
TI **Crystal** and molecular structure of aminoguanidine sulfate, an important enzyme inhibitor and starting material of drug syntheses
AU Koskinen, Mikko; Mutikainen, Ilpo; Elo, Hannu
CS Dep. Pharm., Univ. Helsinki, Helsinki, FIN-00014, Finland
SO Zeitschrift fuer Naturforschung, B: Chemical Sciences (1994), 49(4), 556-60
CODEN: ZNBSEN; ISSN: 0932-0776
DT Journal
LA English
AB Aminoguanidine is not only an agent with a variety of pharmacol. effects but also an important starting material of amidinohydrazone-type drugs and enzyme inhibitors. Therefore, the authors have now synthesized aminoguanidine sulfate CN4H82+.SO42- and detd. its structure by single-**crystal** x-ray diffraction. The doubly protonated (dication) form of aminoguanidine that is present in the sulfate could, in principle, exist as several different tautomers. The **crystal** studied consisted exclusively of 1 tautomer: 1 of the nitrogens of the hydrazine moiety bears 3 hydrogen atoms while the other 1 (the 1 bound to the C) bears 1 H. The other 2 nitrogens are bound to 2 hydrogens each. The predominance of this tautomer can be explained by the very strong resonance in it. The dication of aminoguanidine is remarkably planar. The hydrogens of the hydrazine moiety are, however, clearly out of the plane of the other atoms. There is a strong H bond between the proton of the monoprotonated nitrogen and 1 sulfate O. This bond obviously causes the deviation of the H from the plane. The bonds between the C atom and the adjacent nitrogens are essentially equally long, indicating that each bond has approx. the same amt. of double bond character. One of the pos. charges of the dication is thus delocalized, being shared by all of the atoms of the CN3 moiety. In this respect, the structure is similar to that of all bis(amidinohydrazones) whose structures were detd. The other pos. charge of the aminoguanidine dication is localized at the nitrogen bearing 3 hydrogens.

L3 ANSWER 19 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1994:106940 CAPLUS
DN 120:106940
TI Diels-Alder reactions of 1,2,4-triazines with cyclic vinyl ethers
AU Gonsalves, Antonio M. d'A. Rocha; Pinho e Melo, Teresa M. V. D.;

Gilchrist, Thomas L.
CS Fac. Cienc. Tecnol., Univ. Coimbra, Coimbra, P-3049, Port.
SO Tetrahedron (1993), 49(24), 5277-90
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
OS CASREACT 120:106940
GI



AB The Diels-Alder reaction of cyclic vinyl ethers I (n = 2, R = H, OMe, OEt; n = 1, R = H) with 1,2,4-triazines II (R1 = R2 = Ph, CO2Et, R3 = NH2, NHAc, Me, CO2Et; R1 = H, R2 = Ph, R3 = CO2Et) leads to a range of substituted pyridines with hydroxyalkyl and oxoalkyl side chains. With dihydrofuran, aromatization of the 1:1 adduct is inhibited by conformational factors and this allows 2:1 adducts to be isolated. Different regioselectivity is obsd. in the 2:1 adducts formed from II (R1 = H, Ph, R2 = Ph, R3 = CO2Et). An x-ray **crystal** structure of the 2:1 adduct III, formed from 2,3-dihydrofuran and II (R1 = R2 = Ph, R3 = CO2Et), is reported.

L3 ANSWER 20 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:592717 CAPLUS
DN 113:192717
TI Bonding of fluoropolymers which are not melt-processable to dimensionally stable composite components
IN Schmidt, Erich; Zipplies, Tilman
PA Hoechst A.-G., Germany
SO Ger. Offen., 8 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE 3840514	A1	19900607	DE 1988-3840514	19881201
PRAI DE 1988-3840514		19881201		

AB In the title process, which is economical, the solid, powd. fluoropolymers are mixed with alkali metal or alk. earth salts of cyanamide; ammine complex salts of Cr and Group IB, IIB, or VIIIB metals; HH4 salts of H2CO3, carbamic acids, or carboxylic acids; or other compds. which cleave NH3 at 80-400.degree. (contg. .gtoreq.15% N) and pressed with the other composite component at 5-50 MPa and temps. between the fluoropolymer **crystallite** m.p. and 400.degree.. PTFE (av. particle size 30 .mu.m) contg. 2% hexamethylenetetramine (I) (particle size <125 .mu.m) was pressed at room temp. and 5 MPa to a 50-.mu.m film which was pressed between glass plates at 380.degree./113.8 MPa to give a composite with adhesion 920 .+-. 50 N; vs. 360 .+-. 40 without I.

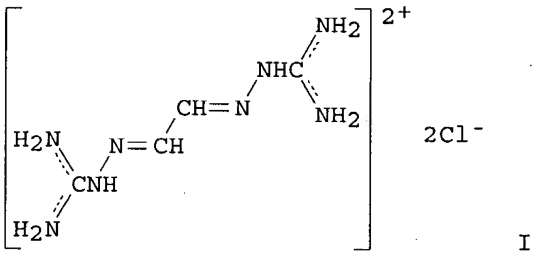
L3 ANSWER 21 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1988:563047 CAPLUS

DN 109:163047
TI Biochemical and chemical characterization of trifluoromethylglyoxal bis(guanylhydrazone), a close analog of the antileukemic drug mitoguazone
AU Elo, Hannu; Mutikainen, Ilpo
CS Dep. Chem., Univ. Helsinki, Helsinki, SF-00100/10, Finland
SO Zeitschrift fuer Naturforschung, C: Journal of Biosciences (1988), 43(7-8), 601-5
CODEN: ZNCBDA; ISSN: 0341-0382
DT Journal
LA English
AB Trifluoromethylglyoxal bis(guanylhydrazone) (CF3-GBG), a close analog of the antileukemic drug methylglyoxal bis(guanylhydrazone) (mitoguazone, MGBG) was synthesized according to a novel modification of previous methods, yielding single **crystals**. Single-**crystal** x-ray **crystallog**. revealed the presence of an isomer different from the one detected in the case of MGBG and all other bis(guanylhydrazones) so far studied. In contrast to MGBG, CF3-GBG was a very weak inhibitor of yeast adenosylmethionine decarboxylase, being thus devoid of value as a polyamine antimetabolite. In addn., the compd. did not have antiproliferative activity against mouse L1210 leukemia cells in vitro. As long as analogous isomers of the 2 compds. are not available, no conclusions can be drawn about the reasons lying behind the drastic differences between their biol. properties.

L3 ANSWER 22 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1987:29203 CAPLUS
DN 106:29203
TI Biochemical properties and **crystal** structure of ethylmethylglyoxal bis(guanylhydrazone) sulfate - an extremely powerful novel inhibitor of adenosylmethionine decarboxylase
AU Elo, Hannu; Mutikainen, Ilpo; Alhonen-Hongisto, Leena; Laine, Raija; Janne, Juhani; Lumme, Paavo
CS Dep. Chem., Univ. Helsinki, Helsinki, SF-00100, Finland
SO Zeitschrift fuer Naturforschung, C: Journal of Biosciences (1986), 41(9-10), 851-5
CODEN: ZNCBDA; ISSN: 0341-0382
DT Journal
LA English
AB Ethylmethylglyoxal bis(guanylhydrazone) (EMGBG) sulfate, an analog of the well-known antileukemic drug methylglyoxal bis(guanylhydrazone), was synthesized. It is an extremely powerful competitive inhibitor of eukaryotic S-adenosylmethionine decarboxylase, with an apparent Ki of 12 nM. Thus, it appears to be the most powerful known inhibitor of the enzyme, being almost an order of magnitude more powerful than the corresponding ethylglyoxal deriv. It neither inhibited the proliferation of mouse L1210 leukemia cells in vitro, nor potentiated growth inhibition produced by .alpha.-difluoromethyl ornithine. In this respect, its properties are closely related to those of dimethylglyoxal, ethylglyoxal, and propylglyoxal bis(guanylhydrazones), but are in striking contrast to those of the antiproliferative glyoxal and methylglyoxal analogs. EMGBG also inhibited intestinal diamine oxidase activity (Ki 0.7 .mu.M). EMGBG sulfate was crystd. from water, giving orthorhombic **crystals** (space group Pbcn). The **crystal** and mol. structures was detd. by x-ray diffraction methods. The C:N bonds between the ethylmethylglyoxal part and the aminoguanidine moieties had the same configuration as they are known to have in the salts of glyoxal, methylglyoxal, and propylglyoxal bis(guanylhydrazones). The glyoxal bis(guanylhydrazone) chain of the EMGBG cation deviated strongly from planarity, thus differing dramatically from the corresponding chains of the glyoxal, methylglyoxal, and propylglyoxal analogs.

L3 ANSWER 23 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1986:206697 CAPLUS
DN 104:206697

TI **Crystal** and molecular structure of glyoxal bis(amidinohydrazone) dihydrochloride; biochemical aspects
AU Mutikainen, Ilpo; Elo, Hannu; Lumme, Paavo
CS Dep. Chem., Univ. Helsinki, Helsinki, SF-00100, Finland
SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1986), (2), 291-3
CODEN: JCPKBH; ISSN: 0300-9580
DT Journal
LA English
OS CASREACT 104:206697
GI



I

AB The **crystal** and mol. structure of the title compd. (I) was detd. by x-ray anal. The structure consists of layers of dipos. cations [C4H12N8]2+ and Cl- ions. The planar cation has the trans configuration of the chain. H bonds of the type N-H...Cl- are formed within the layers, but not between them. The mols. in the **crystal** are held together through stacking and via the delocalized .pi.-electron system. The mean planes of the cations are .apprx.3.51 .ANG. apart. The **crystal** structure is compared with that of other bis(amidinohydrazone) derivs. and the relationship between **crystal** structure and biochem. properties is discussed.

L3 ANSWER 24 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1965:469025 CAPLUS
DN 63:69025
OREF 63:12660e-g
TI Synthesis of aminoguanidine bicarbonate
AU Spiliadis, A.; Hilsenrath, Melania; Molau, Gheorgheta
SO Revistade Chimie (Bucharest, Romania) (1965), 16(6), 328-31
CODEN: RCBUAU; ISSN: 0034-7752
DT Journal
LA Romanian
AB A detailed study of the synthesis of aminoguanidine bicarbonate, based on the condensation of neutral hydrazine sulfate with cyanamide, gave the following optimum reaction conditions. A 9.8% H2NNH2.H2SO4 soln. (8.3 moles) was added to a 4% H2NCN soln. (11.25 moles) at pH 5-6, so that the pH decreased to <3.5, and NaHCO33 (800 g.) was added gradually, while stirring, keeping the foam at a min. until pH 5-6 was attained. When the suspension passed into soln. (sol. (H2NNH2)2H2SO4 was formed), boric acid (340 g.) was added (to a 3% concn. with respect to the H2O), and the mixt. was refluxed at pH 7.3-7.2. After cooling the soln., aminoguanidine sulfate was sepd. from the small amt. of ppt. salts by filtration. The filtrate was purified with activated charcoal at 80.degree., adding NaHCO3 (1.2 kg.) while hot, and cooling to 10.degree.. The aminoguanidine bicarbonate pptd. as white **crystals** within 3 hrs. The cake contg. 63% the product, the rest being H2O and NaHCO3, was used to prep. 3-amino-1,2,4-triazole. The conversion of the H2NNH2.H2SO4 was 96% and the yield with respect to it was 96%. When operating at lower temps. (90.degree.) the reaction duration was of the order of hrs. The pH at the reflux temp. affected considerably the reaction yield, and the reaction

rate, which increased with the pH up to 7.2-7.3. However, above pH 7.3 the cyanamide degradation rate increased appreciably. The use of boric acid to attain this optimum pH was based only on its buffering effect and not on a possible cyanamide stabilization.

L3 ANSWER 25 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1964:90316 CAPLUS
DN 60:90316
OREF 60:15728g-h
TI Preparation of guanidine malonic acid salt
AU Brudz, V. G.; Rozina, D. Sh.; Nesterenko, L. T.
SO Metody Polucheniya Khimicheskikh Reaktivov i Preparatov (1962), No.4-5, 20-1
CODEN: MPRPAT; ISSN: 0539-5143
DT Journal
LA Unavailable
AB In 1 hr. 208-10 g. malonic acid (I) was added with mixing to a soln. of 182 g. guanidine carbonate in 560 ml. distd. H2O at 55-60.degree. and kept weakly acidic by the addn. of more I if necessary while stirring an addnl. hr. Activated C (5 g.) was added, the soln. mixed 15 min. and filtered, and the filtrate cooled to 20.degree. and allowed to **crystallize** 5 hrs. The needles were filtered, press-dried, and combined with the addnl. material obtained by repeated concns. of the mother liquor on a steam bath and cooling to 15-20.degree.. The combined product was dried at 90-5.degree. to yield 239-47 g. of 99.2-9.8% pure guanidine malonic acid salt, m. 151-1.5.degree. (alc.).